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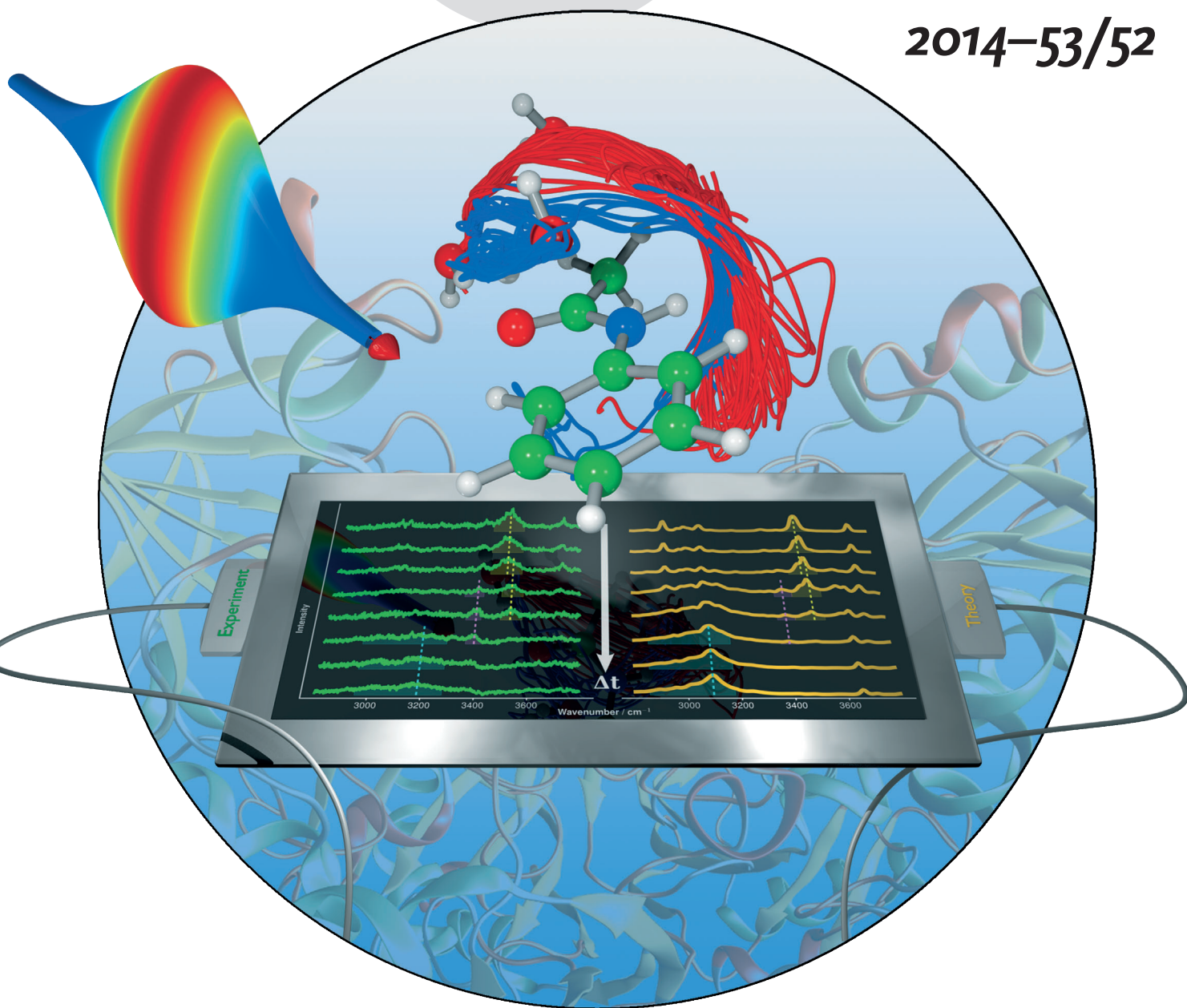
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Simulations of water solvation dynamics ...

... around biomolecular structures can be verified reliably by experimental time-resolved IR spectroscopy. In the work of a German–Japanese collaboration headed by O. Dopfer, M. Fujii, and R. Mitric and reported in a Communication on page 14601 ff., the approach was applied to the acetanilide–water cluster. Photoionization triggers the migration of a water molecule from the CO to the NH group of the amide by both a fast (red) and a slow (blue) reaction path.

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